The National Energy Technology Laboratory

Office of Coal and Power R&D

Technology Plan: Coal Fuels

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Coal Fuels and Hydrogen

Currently, the United States imports approximately 11 million barrels per day of petroleum crude and finished products (55% of consumption). By 2020 imports are projected to rise to 17.5 million barrels per day of crude and refined products (67% of consumption). The Middle East

will provide the bulk of the exportable petroleum crude since that region contains 75% of the world's reserves. Imports of Middle East (ME) oil from these sources represent about 2.2 MMBPD at present but are expected to increase to over 5 MMBPD by 2020. Coal-derived fuels, especially hydrogen, can be an important part of a strategy to diversify and expand our domestic fuel resource base, as well as helping to limit our reliance on imported oil by expanding our use of domestic resources

In addition to energy security issues, major challenges facing transportation are urban and regional air pollution and emissions of greenhouse gases. Of the man-made emissions, U.S. transportation is responsible for nearly 80 percent of the carbon monoxide (CO), over one half of the nitrogen oxides (NOx), and 40 percent of the volatile organic compounds (VOC). Vehicles are responsible for about 35% of the U.S. energy sector's carbon dioxide production. As the Nation transitions toward ultra-low emissions vehicles and eventually zero emissions vehicles, such as the Administration's recently announced initiative to develop the fuel cell-powered "Freedom Car", there will be a need to develop clean fuels for both of these scenarios. Our large domestic resources of coal can provide ultra-pure hydrogen for fuel cells and ultra-clean, high performance liquid fuels for advanced engine/after-treatment systems as well as liquid hydrogen carriers for reforming applications on-board or off-board the vehicle.

Our Current Situation

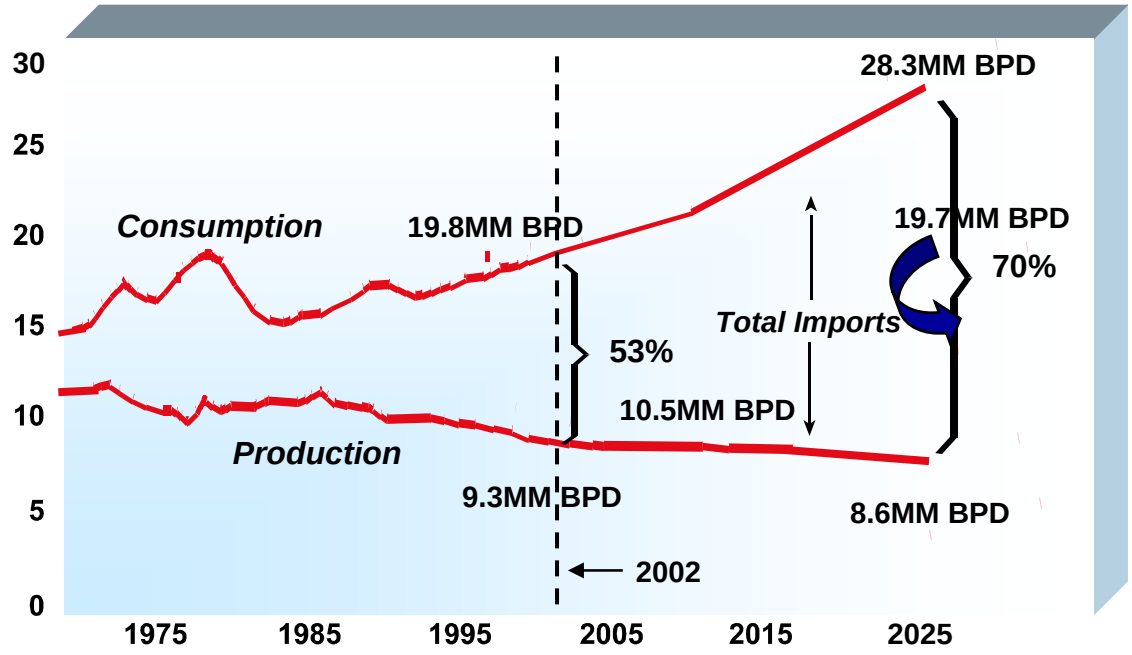
Our National Security is threatened by increasing dependence on imported petroleum from unstable world regions

Experts predict world oil production will peak in first half of this century

Transportation is a major contributor to regional air pollution and ultra clean fuels are essential to mitigate this (CO 80%, NOx 50%, VOC 40%)

Transportation is responsible for one-third of U.S. greenhouse gas emissions (~500 MMT)

Affordable transportation is essential for our continued economic prosperity



In addition to premium liquid fuels and hydrogen, coal presents unique opportunities to produce other high value products. Coal can be used to make high purity carbon electrodes and specialty graphites that are better quality than those made from conventional processes that rely on petroleum coke. Composite fuels comprised of coal and waste biomass can help offset the release of greenhouse gases during combustion. Throughout the U.S. coal producing regions, there are large amounts of coal residing in waste ponds. Separation processes to economically recover the coal could make it available for power generation and, concurrently, eliminate existing and potential environmental problems associated with these waste sites.

NETL recognizes the need to make the United States less vulnerable to international energy crises and fuel shortages, improve the environmental performance of every component in the fuels production, processing, delivery, and utilization chain, and make possible a significantly cleaner and more efficient transportation fleet. Subsequently, we have developed partnerships with other government agencies and all elements of the fuels and transportation industries, including fuel producers, technology developers, and engine and emission control manufacturers. In conjunction with these partners, we have designed our fuels RD&D programs to address the issues that industry and our nation face.

Transportation Fuels & Chemicals

Research efforts are focused on developing technologies for making clean liquid fuels, hydrogen, and fuel additives and lubricants from domestic coal-derived synthesis gas. The outcome of these research efforts will help provide the transportation sector with significant environmental benefits and help to diversify our domestic resource base for the production of fuels.

DOE-sponsored research to produce liquid fuels from coal has resulted in a series of advances that have enabled the United States to remain competitive in the international arena. Many

countries, including Germany, Japan, South Africa, and the Netherlands, have vigorously pursued synthesis gas conversion research based on both coal and stranded natural gas feedstocks. U.S. – industry partnered R&D efforts that began after World War II to produce liquid fuels from coal-derived synthesis gas have assisted efforts to develop economic approaches to convert natural gas to liquid fuels, known as "gas-to-liquids" (GTL) technology. Many U.S. firms are currently planning to deploy GTL technology for the near- to mid-term markets, whereas coal - derived fuel technologies are viewed as being deployed longer-term because extensive research is needed to reduce costs, minimize greenhouse gas emissions and ensure the plants meet strict environmental requirements for pollutant emissions.

Hydrogen has been recognized for many years as the premier fuel for emissions-free transportation. In early 2002 the Administration announced the "Freedom Car" initiative, which has lent even greater interest in pursuing the research needed to satisfy the demands of future hydrogen-fueled, fuel cell powered vehicles. Subsequently, the Department announced a complementary, Hydrogen Fuel Initiative in early 2003 followed by plans to build a prototype coal-fired power plant of the future ----termed FutureGen that will combine electricity and hydrogen production with the virtual total elimination of harmful emissions, including greenhouse gases.

Coal contains the largest domestic resource of hydrogen but significant issues must be addressed to ensure that coal-derived hydrogen is produced, delivered and stored in a manner that is safe, environmentally acceptable and economic.

Progress to Date

The **Transportation Fuels and Chemicals** program encompasses a broad range of activities designed to provide the technical means to produce liquid fuels and hydrogen from coal. This program involves investigations that range from laboratory-scale studies of new fuel-making concepts to, until recently, proof-of-concept testing at the Alternative Fuels Development Unit (AFDU) located in La Porte, TX and operated by Air Products and Chemicals, Inc. (APCI). Due to the Adminstration's strong emphasis on hydrogen research, it has been decided to close and dismantle the facility in calendar year 2005. However, the AFDU has a long history of successes which have advanced significantly the development of technologies to produce clean fuels from coal. The plant used synthesis gas (hydrogen and carbon monoxide) from a nearby APCI facility as the reactant for producing a wide range of high value products in quantities up to 35 barrels per day. The specific product slate is determined by:

La Porte AFDU

the hydrogen to carbon monoxide ratio of the synthesis gas,
the reactor operating conditions, and
the catalyst used.

The Department of Energy, in collaboration with APCI, operated the AFDU from 1981 through 2002 for a host of applications. As examples, the development work that concluded in 1990 for Liquid Phase Methanol™ technology led to its highly successful demonstration and continued operations that produce over 300 barrels per day at Eastman Chemical's Kingsport, TN facility. More recently, a novel process to produce an alternative diesel fuel (dimethyl ether) has been evaluated and two oil companies utilized the AFDU to evaluate advanced Fischer-Tropsch processes.

In 1998, the coal fuels research effort was enhanced through a joint effort with the Gasification Technology Systems product line to sponsor the development of technology that coproduces some combination of power, fuels and chemicals. Coproduction involves the integration of: coal gasification to produce synthesis gas; conversion of a portion of the synthesis gas to high-value fuels and/or chemicals; and combustion of the remaining synthesis gas to produce electric power. This strategy makes more efficient use of capital than producing power alone. Also, the amounts of power and fuel produced will be dictated by market demands. The industry-led WMPI coproduction team completed its technical-economic analyses and R&D tasks needed to reduce the risk of integrating the fuel and power systems. Government sponsorship will conclude in 2005 with preparation of preliminary engineering designs for the plant concept. As a next step toward commercial reality, WMPI proposed a follow-on effort that was selected in early 2003 in response to the Department's Clean Coal Power Initiative. The proposed $612 million project would culminate in design, construction and operation of a plant in northeast Pennsylvania that would use anthracite waste to co-produce electricity, high-value industrial heat and 5,000 barrels per day of ultra-clean burning diesel fuel.

As the coal fuels program moves toward greater emphasis on hydrogen, detailed analyses will be performed for "hydrogen from coal" system options that lead to specific research recommendations. In addition, the Department commissioned the National Academy of Sciences to investigate "The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs." The final report is available at www.nap.edu. Among many comments and recommendations, the Academy noted that: "The U.S. has vast coal resources…hydrogen from coal can be inexpensive…and…coal must be a significant component of R&D aimed at making very large amounts of hydrogen." The output of this study will help construct research paths for producing hydrogen from all sources, including fossil, renewable and nuclear.

NETL on-site researchers have constructed and are operating a unique, very versatile membrane test unit that enables manufacturers to quickly test hydrogen separation membranes over a wide range of temperatures and pressures and subsequently do detailed analyses of the effect of operating conditions on the membrane. The unit and the research team are an important component in the nation's move toward greater hydrogen utilization.

On of the key steps in producing hydrogen from coal is separating it from the many other gases that are produced in the gasification process. Because of this, hydrogen separation membranes and other potential separation technologies are a key component to enable economic, widespread use of hydrogen in fuel cell- powered vehicles and stationary, distributed power systems. Further, once a pure stream of hydrogen is obtained, there are added technical challenges associated with storing, handling and transporting the hydrogen in a manner that provides the customer with safe, affordable fuel. Alternatively, high hydrogen content coal liquids may provide a nearer-term path to the hydrogen economy by using the existing fuel distribution network and reforming the liquids at or near the point of use. All these research elements are included in the evolving hydrogen from coal research, to an extent determined by our internal systems engineering analyses and external feedback from the research community. Implementation of a comprehensive hydrogen from coal research program began in FY 2003 through the selection of five projects in NETL's Broad-Based solicitation for hydrogen separation. The FY 2004 solicitation enabled the program to expand the research efforts into the utilization of hydrogen and natural gas mixtures in internal combustion engines. Again, this approach may facilitate the use of hydrogen near term, until fuels cells become commercial.

The ultimate success of any fuel development effort depends on the vehicle performance. However, the fuel only represents one side of the fuel-engine-aftreatment triangle. Partnerships

have been created with the Department of Defense (DOD) which is particularly interested in Fischer-Tropsch fuels that can offer high performance and low emissions for ground, air and marine applications. NETL on-site researchers are working on joint projects with the Air Force and Army to address their specific technical issues, such as fuel lubricity and fuel quality when exposed, for example, to the rigorous demands of high performance aircraft.

Planned Activities

The La Porte AFDU and research associated with the facility has been completed. Specifically, the process to eventually dismantle the AFDU and restore the site began in FY 2004. The newly configured coal fuels research will embody a program structure that incorporates important elements directly related to meeting the Office of Fossil Energy's goal of "Promoting the development and deployment of technologies that produce clean, high performance liquid and gaseous fuels from a variety of secure energy resources." Some specific aspects of our strategy to meet this goal include:

Implement external research targeted at: a) developing hydrogen technology modules that will be available for the FutureGen plant and b) adding to the scientific base needed to distribute the hydrogen produced at the this plant and future commercial operations.

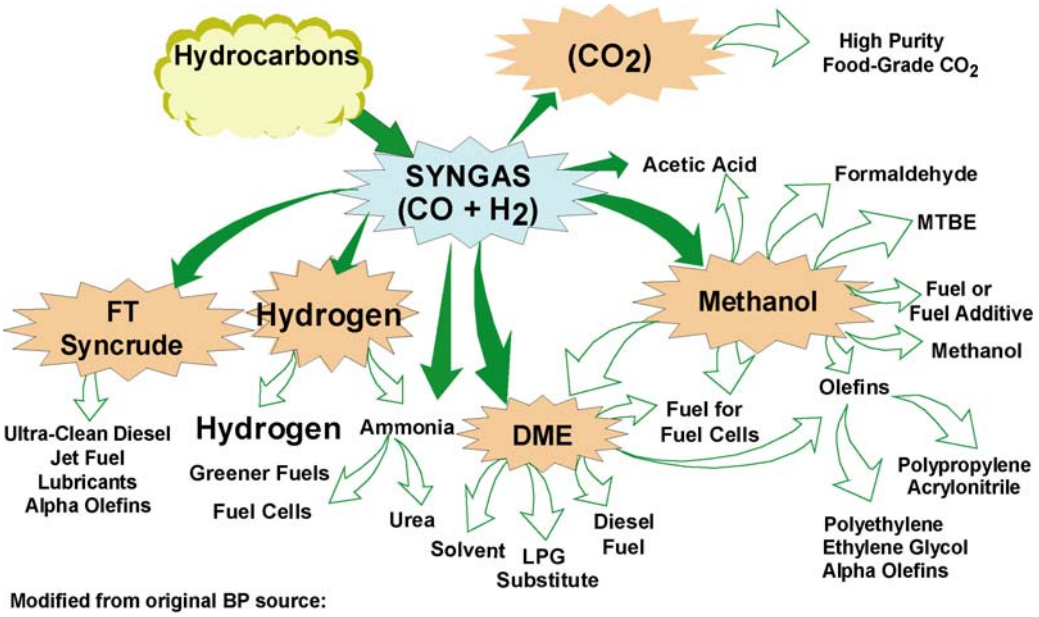
Direct the NETL Ultra-Clean Fuels Focus Area to research that will facilitate the deployment of fuel cell - and internal combustion - powered vehicles; and apply computational fuel science that offers step-out advances in the design of coal fuels processes and significant reductions in technology development time and costs.

Complete the WMPI Early Entrance Coproduction project to ensure a smooth transition into the CCPI demonstration. If successful, this effort could provide an important step toward showing that coal can help achieve the Nation's energy goals by producing a market-driven combination of clean products, including hydrogen.

Strengthen our collaborations with the military by evaluating coal-derived liquid fuels and hydrogen for strategic military applications and determining their capability to enhance operational readiness.

Legacy Activities

Although the emphasis of this Technology Plan is Coal Fuels, there are some projects initiated under a number of programs that used simpler hydrocarbons than coal as starting feedstock for conversion to synthesis gas Congress directed that a Hydrogen from Natural Gas program be delayed until FY05 (or later) and that limited funding be directed to continuing and finishing up projects previously in the Advanced Synthesis Gas, Clean Fuels, Petroleum Fuels program. Some reasons for these programs were monetization of stranded natural gas; development of more efficient membrane technology to produce synthesis gas and liquid fuels, including F-T diesel fuel which has environmental premiums associated with its use; and scoping of ideas or solving fundamental problems within DOE's National Laboratories to catalytically convert methane to higher value products. Five projects were reviewed by industry as part of the June 4-5, 2003 Merit Review of Advanced Synthesis Gas and Clean Fuels projects. A summary of the Merit Review is Appendix A in the FY04 Petroleum Fuels Product Plan.



Eleven projects will continue in FY05 either through FY05 funds or from FY04 funds as well as Small Business Innovative Research projects (two phase II and seven phase I on natural gas to hydrogen or membranes research – individual descriptions not included). Specific projects that are expected to continue using FY05 funds include: Air Products and Chemicals, ICRC/Syntroleum and ConocoPhillips. Projects use natural gas as feedstock and include membranes research and research on conversion of synthesis gas. The University of Alaska oxygen transport ceramic membrane project is funded through the Arctic Energy Center. Projects are briefly described below:

APCI, three-phase effort directed to development of a novel ceramic membrane reactor able to separate oxygen from air and partially oxidize natural gas to synthesis gas in a single step. APCI, a leading industrial gas producer, is undertaking this "Ion Transport Membrane (ITM) Syngas" research effort. This technology will provide the benefits of using pure oxygen for synthesis gas production while avoiding the expense of a separate air separation plant. This could reduce F-T fuel costs by as much as 25%.

- University of Alaska is working with a number of companies including Alyeska Pipeline to investigate the operational challenges in using the TransAlaska Pipeline System for transporting GTL products.
- University of Alaska with Praxair as part of the industrial team will continue their development of a second approach – oxygen transport ceramic membrane technology for conversion of natural gas to F-T fuels.

Three projects within FY04 Petroleum Fuels Program, Clean Fuels Subprogram were being finished up in late FY04 or had extensions to complete. These projects supported investigation of other synthesis gas generation approaches, F-T catalyst studies, and other process improvements and alternatives. Projects are briefly described below:

ICRC/Syntroleum: Continued operation of a 70 barrel/day pilot small footprint GTL plant

and fleet test of F-T fuels.

Praxair: Development of oxygen transport membrane materials and reactor designs and complete engine testing/development using F-T fuels.

ConocoPhillips: Evaluate the economics of GTL as well as potential F-T fuel markets and field test fuels using commercial fleets of ignition compression engines, fuel cell vehicles and a turbine for alternative use of the ultra clean fuels for power generation.

Five projects are being conducted at DOE's National Laboratories. Projects are briefly described below:

INEEL: Evaluation of catalytic methane decomposition for the production of hydrogen and solid carbon without partial oxidation or production of carbon dioxide.

NETL: Multipart project to examining the feasibility of novel "dry reforming" of CO_2 to make synthesis gas; development of attrition-resistant F-T catalysts, and development of catalysts to extract hydrogen and sulfur from H_2S and H_2S-containing waste gases.

NETL: Develop system for capturing CO_2 from the exhaust gas streams when natural gas is converted to synthesis gas or reformed synthesis gas with major commercial product being hydrogen.

NETL: Develop metal organic frameworks having appropiate pore dimensions and surface properties to enhance separation and storage properties with the objective of searching for materials that facilitate separation of CO_2 from natural gas.

NETL: Seek to understand the mechanism of sulfur resistance (sulfur poisioning of surfaces that shortens the life of membranes and catalysts) of Pd-Cu membranes. This could provide the foundation for understanding membrane poisoning from other impurities.

Advanced Fuels Research

The **Advanced Fuels Research** program acts as a bridge between basic and applied research and meets two major needs. The first is the basic information and knowledge needed to surmount technical barriers encountered by the fuels research programs. The second is the exploration and evaluation of innovative concepts and ideas that anticipate requirements and advances in fuel formulations and fuel use technologies that, if successfully developed, would enhance the overall pace of technology development. Both needs could be met by developing a readily transferable knowledge base of the chemical and physical processes underlying advanced technologies. This "supporting science" will address key technology barriers, R&D opportunities, and research requirements.

Progress to Date

Key areas shaping the Advanced Fuels Research program include several projects at the Consortium for Fossil Fuels Science (CFFS) that focus on the production, purification, and storage of hydrogen produced from coal and the use of "C-1" chemistry to produce environmentally desirable fuels and fuel additives. The ability to produce hydrogen from coal with minimal emissions early in a transition to a so-called "hydrogen economy" would help to facilitate this transition by the promoting the continued use of fossil fuels. Work in synthesis gas chemistry, the computational chemistry of the many aspects of fuels production, and methods for the rapid screening of desulfurization processes are being pursued.

"C-1" chemistry is defined as the chemistry of compounds containing a single atom of carbon. The C-1 compounds of greatest interest to the Department are methane, carbon monoxide, carbon dioxide, and methanol. An understanding of the chemical and physical processes needed to transform these compounds into various fuels and fuel additives that could be produced from domestic resources would provide significant environmental benefits. The most comprehensive work in this area is being carried out by the CFFS, a research consortium with participants from the University of Kentucky, West Virginia University, the University of Utah, the University of Pittsburgh, and Auburn University. This consortium has enlisted the help of an Industrial Advisory Panel which tempers the academic research with first hand knowledge of industry concerns and needs. The consortium pursues catalyst development and investigates the chemistry of Fischer-Tropsch (F-T) fuels, methanol, complex oxygenate synthesis, oxygenated additives for gasoline and diesel, hydrogen production, and synthesis gas production.

NETL on-site researchers are evaluating the properties of carbon and metal-organic materials to determine their potential for use as hydrogen storage media. Potentially, these novel materials could provide safe, high capacity hydrogen storage for fuel cell powered vehicles.

A project at West Virginia University (WVU) is closely tied to the research being performed at the Consortium for Premium Carbon Products from Coal (CPCPC) which is described in the Solid Fuels and Feedstocks program activities. The objective of the WVU effort is to perform laboratory research in the area of extracting hydrocarbon materials from coal that can subsequently be used by the CPCPC to develop processes for making high-value products. Specifically, the coal extraction process holds promise as a cost-competitive source of improved binder pitch, carbon fibers, and carbon structural foams. Coal tar pitch, the binder commonly used in anode production and other carbon materials applications, is now a byproduct that is generated during coke production. Because of aging coke batteries, a declining steel industry, and more stringent environmental regulations, the continued availability of sufficient tar of the required quality is in doubt. The coal extraction process under development uses a recoverable solvent to extract a material from bituminous coals that is similar in properties to coal tar pitch. The production of a consistent, high-quality product is a key advantage of extraction methods for making pitch precursors from coal. Other products that could result from this approach include (1) binders, (2) mesophase and isotropic pitches (as carbon foam and fiber precursors), (3) coker feedstocks (for needle, sponge, and specialty cokes), and (4) impregnation pitches. At this time, the process is being scaled up to demonstrate the technology and generate enough extract to determine its suitability to produce other products.

Planned Activities

The aforementioned research at the CFFS and WVU is being continued in FY 2005. In accordance with the Department's focus on hydrogen research, the CFFS will place increased emphasis on developing the science base for producing hydrogen from coal.

Solid Fuels

The goal of the Solid Fuels program is to provide the scientific and engineering knowledge base that could enable industry to produce economically competitive and environmentally acceptable products and feedstocks from coal and mixtures of coal and other resources.

The Consortium for premium Carbon Products from Coal (CPCPC) is performing research in a number of areas direct toward making high value materials from coal. Currently, petroleum is used to produce most high-volume and high-value carbon products. The manufacture of electrodes, which are made by graphitization of "petroleum coke" impregnated with pitch, requires a coke having minimal impurities. However, the quality of petroleum feedstocks has declined over the past few years, resulting in more metallic impurities in the coke, which in turn produces a poorer quality electrode. As an example, an electrode with high quantities of vanadium that is used to process steel will change the quantities of vanadium in the product in an unpredictable fashion. As refiners try to extract more liquid products from their crude, the quality of the petroleum residuum (the source of pitch) continues to decline. All ranks of coal (anthracite, bituminous, sub-bituminous, and lignite) could prove to be good feedstock substitutes for petroleum-based materials for the manufacture of premium carbon products. Coal-derived specialty graphites are considered to have higher purity, strength, and isotropy that those derived from petroleum. Anthracite offers promise because of its high carbon and low sulfur and ash content and high volatile bituminous coal shows promise as a source for binder pitch when extracted with appropriate solvents. Once low cost processing technologies are developed, coal will naturally find uses in other carbon products because of its surety of supply and widespread availability.

Advanced separation technologies will allow companies to extract, process, and dispose of coal and mineral substances without objectionable social and environmental costs, and to reclaim valuable resources from wastes. Many of the advanced separation technologies to be developed by the Consortium for Advanced Separation Technologies will have cross-cutting applications to a variety of other industries.

Progress to Date

The **Solid Fuels** program is conducting research in the following areas:

Premium Carbon Products
Integration of a Coal Fuels Process into an Operating Refinery
Advanced Separations Technology for Mining and Minerals Applications.

Pennsylvania State University is leading the Consortium for Premium Carbon Products from Coal. This activity involves a unique, industry driven consortium, whose nearly 50 industrial and academic members identify, select, and co-fund research initiatives that are focused on producing value-added carbon products. The industrial members often partner with academic institutions in cost-shared (the private sector provides at least half of the funding) research projects that look to commercialize carbon products derived from coal. The projects sponsored by the consortium are diverse and broad in scope. As an example, one project demonstrated the ability to reactivate carbon adsorbents used to purify drinking water at the Cincinnati Waterworks.

Advanced separations technology is being applied to dewatering coal fines to allow the recovery of coal from settling ponds as a fuel and eliminate the need for these ponds and the environmental hazard they pose in the future. Furthermore, technology is being developed to separate carbon particles from power plant fly ash. The installation of approaches to reduce NO_x emissions at power plants changes the characteristics of the fly ash collected. If the carbon particles remain in the fly ash, beneficial uses of the fly ash (e.g., to make cement) would no longer be possible. Instead, the fly ash containing carbon particles would require disposal as a waste material in a landfill. Removal of these carbon particles also produces a high-surface-area carbon that could be used as a sorbent to reduce air toxics emissions, such as mercury, from power plants.

Planned Activities

The Center for Advanced Separations Technology (CAST) located at Virginia Tech and West Virginia University provides the scientific basis for development of advanced solid-solid and solid-liquid separation technologies important to the Mining and Minerals industry. One of the focus research efforts is directed toward dewatering of coal fines settling ponds to serve the dual purposes of recovering a low cost coal resource, while eliminating the environmental issues associated with coal waste ponds. Technology is also being developed to recover power plant fly ash from settling ponds. Recovery includes separation of the flyash into several distinct product streams, including two carbon streams for fuel or sorbent use, and several mineral streams for resale to the cement industry.

The Consortium for Premium Carbon Products from Coal (CPCPC) will continue to match industry needs with university researchers in efforts to expand the uses of coal. New work will include developing technologies to produce coal-derived carbon fibers for high-strength composites, foams for high temperature insulation and electrodes, activated carbons for water purification and mercury capture, coal-metal composites for hydrogen storage, carbons for fuel cell applications and coal-based biological production of hydrogen. At the October, 2003 CPCPC workshop, eleven projects in these areas were selected for funding in FY04.

A project that began in September, 2003 addresses direct coal conversion technology. Specifically, Pennsylvania State University (PSU) is attempting to optimize the value of all product streams resulting from processing coal to make, primarily, a jet fuel fraction. Besides the jet fuel, which has similarities to diesel fuel and kerosene, other hydrocarbon streams are produced that need to be processed/refined to ensure a maximum value of the entire product mix. The University will be working with a refiner to develop a strategy that accomplishes this goal.

The “Hydrogen” portion of the Coal Fuels and Hydrogen product line was implemented in FY 2003 and is receiving increasing importance as reflected in the budgets for FY 2004 and FY 2005. The following attachments provide details on the planning, analyses and outreach that are being performed to respond to the Administration’s vision for hydrogen.

1. Fossil Energy Hydrogen Program Plan (includes plans for both coal and natural gas research)
2. Hydrogen from Coal RD&D Plan
3. Mitretek: Hydrogen from Coal (examines the performance and economics of current and advanced technologies to produce hydrogen from coal)
4. Presentation on Hydrogen from Coal at Coal Gen 2004, July 29, 2004
5. Hydrogen from Coal Brochure
6. Program Implementation Plan (PIP)